AUTHOR INDEX TO VOLUME 138

Aguilar, M.A. and F.J. Olivares del Valle, A computation procedure for the dispersion component of the interaction energy in continuum solute–solvent models 138 (1989) 327
Ahuja, S.J., see J.W. Harrell Jr. 138 (1989) 383
Alsanoosi, A.M., see A.J. Horsewill 138 (1989) 179
Andresen, B., see J. Herbich 138 (1989) 105
Anisimov, O.A., see A.V. Koptyug 138 (1989) 173

Balasubramanian, K., see P.Y. Feng 138 (1989) 89
Barrientos, C., see A. Largo 138 (1989) 291
Baumgärtel, H., see R. Locht 138 (1989) 433
Begtrup, M., see C. Guimon 138 (1989) 157
Bhanuprakash, K., P. Chandra, C. Chabalowski and R.J. Buenker, Theoretical study of the generalized oscillator strength for the A^1B_1–X^1A_1 transition in the water molecule 138 (1989) 215
Billing, G.D., see C. Nyeland 138 (1989) 245
Blanchard, G.J., An MNDO calculational study of selected oxazine, thiazine and oxazone dyes 138 (1989) 365
Brunner, H., see D. Henrich 138 (1989) 203
Buenker, R.J., see K. Bhanuprakash 138 (1989) 215

Campargue, A., M. Chenevier and F. Stoeckel, High-resolution overtone spectroscopy of SiH_4 and $SiHD_3$ ($\Delta v_{SiH}=6$) and CH_4 ($\Delta v_{CH}=5$) 138 (1989) 405
Cao, J.R., J.M. Zhang, X. Zhong, Y.H. Huang, W.Q. Fang, X.J. Wu and Q.H. Zhu, Photofragmentation of vinyl iodide at 248 nm. Heat of formation of vinyl radical 138 (1989) 377
Chabalowski, C., see K. Bhanuprakash 138 (1989) 215
Chandra, P., see K. Bhanuprakash 138 (1989) 215
Chenevier, M., see A. Campargue 138 (1989) 405
Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Semi-local pseudopotential calculations for the potential energies of the CaHe and CaNe systems 138 (1989) 303

Davister, M., see R. Locht 138 (1989) 433
Denzer, W., see R. Locht 138 (1989) 433
Durig, J.R., H.V. Phan and T.S. Little, Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide 138 (1989) 391

Edelstein, N.M., see S. Xia 138 (1989) 255
Evans, D.K., see M. Ivanco 138 (1989) 441

Fang, W.Q., see J.R. Cao 138 (1989) 377
Feng, P.Y. and K. Balasubramanian, The low-lying electronic states of indium trimer 138 (1989) 89
Fernández Sanz, J., see A. Márquez 138 (1989) 99
Finckh, P., H. Heitele and M.E. Michel-Beyerle, Intramolecular electron transfer in viscous solution 138 (1989) 1

Frattini, R., D. Gazzillo, M. Sampoli and R. Vallauri, Analysis of the orientational order induced by different potential models for CO_2 138 (1989) 337
Fritsch, R.H., see D. Henrich 138 (1989) 203
Furukawa, M., K. Mizuno, A. Matsui, N. Tamai and I. Yamazaki, Branching of exciton relaxation to the free and self-trapped exciton states 138 (1989) 423

Galasso, V., Ab initio study of the outer valence ionization potentials and electron affinities of nonconjugated π-electron cyclic systems 138 (1989) 231
Gazzillo, D., see R. Frattini 138 (1989) 337
González, G.G., see A. Márquez 138 (1989) 99
Gracian, F., see C. Guimon 138 (1989) 157
Green, R.M., see A.J. Horsewill 138 (1989) 179
Guimon, C., S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo, HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN_2H_2 energy hypersurface 138 (1989) 157

Haberlandt, H., Pseudopotential MRD CI calculations of nickel-containing molecules. II. The electronic $^1\Sigma^+$ ground state and 20 low-lying excited states of the NiSi molecule 138 (1989) 315
Haley, L.V., see D.L. Thibodeau 138 (1989) 265
Hanson, D.M., see Y. Zhang 138 (1989) 71
Harrell Jr., J.W. and S.J. Ahuja, A relaxation time study of molecular motion in trimethylolpropane triacrylate and trimethylolpropane trimethacrylate 138 (1989) 383
Hashimoto, S., T. Ohba and S. Ikawa, Infrared and molecular dynamics study of reorientational relaxation of liquid acetonitrile 138 (1989) 63
Hausser, K.H., see D. Henrich 138 (1989) 203
Heitele, H., see P. Finckh 138 (1989) 1
Henrich, D., H. Brunner, R.H. Fritsch and K.H. Hausser, Time-resolved microwave-induced optical nuclear polarization 138 (1989) 203
Herbich, J., K. Rotkiewicz, J. Waluk, B. Andresen and E.W. Thulstrup, Transition moment directions and molecular structure of some *p*-cyano-N,N-dimethylaniline derivatives 138 (1989) 105
Hirao, K., see H. Wasada 138 (1989) 277
Horsewill, A.J., R.M. Green and A.M. Alsanoosi, Methyl tunnelling in tiglic acid and 2-methyl-2-butene 138 (1989) 179
Huang, Y.H., see J.R. Cao 138 (1989) 377
Husain, D. and G. Roberts, Time-resolved molecular chemiluminescence investigations of SrO following pulsed dye-laser generation of $Sr(5s5p(^3P_J))$ in the presence of N_2O 138 (1989) 187

Ikawa, S., see S. Hashimoto 138 (1989) 63
Ivanco, M., D.K. Evans and R.D. McAlpine, Multiphoton absorption and luminescence of chromyl chloride 138 (1989) 441

Jayasankar, C.K., see P.S. May 138 (1989) 123
Jayasankar, C.K., see P.S. May 138 (1989) 139
Jochims, H.W., see R. Locht 138 (1989) 433
Jones, A.C., see A.G. Taylor 138 (1989) 413
Jurgis, A.J., see E.A. Silinsh 138 (1989) 347

Kamiya, M., Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model 138 (1989) 11
Khayar, S., see C. Guimon 138 (1989) 157
Kjaergaard, H.G. and O.S. Mortensen, The nature of molecular vibrations selected by various excitation processes 138 (1989) 237
Kleyn, A.W., see E.W. Kuipers 138 (1989) 451
Koningstein, J.A., see D.L. Thibodeau 138 (1989) 265
Koptyug, A.V., V.O. Saik, O.A. Anisimov and Yu.N. Molin, Spin-locking in concentration-narrowed OD ESR spectra 138 (1989) 173
Kuipers, E.W., M.G. Tenner, A.W. Kleyn and S. Stolte, Dependence of the NO/Ag(111) trapping probability on molecular orientation 138 (1989) 451

Largo, A. and C. Barrientos, A theoretical study of the C_2H, C_2F and C_2Cl radicals and their positive ions 138 (1989) 291
Little, T.S., see J.R. Durig 138 (1989) 391
Locht, R., M. Davister, W. Denzer, H.W. Jochims and H. Baumgärtel, About the double ionization of ammonia and carbon dioxide. A comparison between photoionization and electron impact 138 (1989) 433

Márquez, A., G.G. González and J. Fernández Sanz, Ab initio CI calculations on the molecular structure of Sn_2H_4 isomers 138 (1989) 99
Matsui, A., see M. Furukawa 138 (1989) 423
May, P.S., C.K. Jayasankar and F.S. Richardson, Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$ 138 (1989) 123
May, P.S., C.K. Jayasankar and F.S. Richardson, Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$ 138 (1989) 139
McAlpine, R.D., see M. Ivanco 138 (1989) 441
Meister, E.C., see K. Palewska 138 (1989) 115
Michel-Beyerle, M.E., see P. Finckh 138 (1989) 1
Mizuno, K., see M. Furukawa 138 (1989) 423
Molin, Yu.N., see A.V. Koptyug 138 (1989) 173
Mortensen, O.S., see H.G. Kjaergaard 138 (1989) 237
Munn, R.W. and R.J. Phillips, Dielectric theory of weak charge-transfer crystals. III. Dipole moments 138 (1989) 223

Nikitin, E.E. and M.Ya. Ovchinnikova, Optimal trajectory approach in the theory of photodissociation of thermally excited molecules 138 (1989) 45
Nyeland, C. and G.D. Billing, Semiclassical coupled state sudden approximation for multipole cross sections in atom–diatom systems 138 (1989) 245

Ohba, T., see S. Hashimoto 138 (1989) 63
Olivares del Valle, F.J., see M.A. Aguilar 138 (1989) 327
Ovchinnikova, M.Ya., see E.E. Nikitin 138 (1989) 45

Palewska, K., E.C. Meister and U.P. Wild, Spectroscopic evidence for the coexistence of two stereoisomers of tetrabenzonaphthalene in Shpol'skii-type matrices at 4.2 K 138 (1989) 115
Petelenz, P., Charge transfer effects in the pressure dependence of the ultraviolet absorption spectra of polyacene crystals 138 (1989) 35

Pfister-Guillouzo, G., see C. Guimon 138 (1989) 157
Phan, H.V., see J.R. Durig 138 (1989) 391
Phillips, D., see A.G. Taylor 138 (1989) 413
Phillips, R.J., see R.W. Munn 138 (1989) 223
Preuss, H., see E. Czuchaj 138 (1989) 303

Rebentrost, F., see E. Czuchaj 138 (1989) 303
Richardson, F.S., see P.S. May 138 (1989) 123
Richardson, F.S., see P.S. May 138 (1989) 139
Roberts, G., see D. Husain 138 (1989) 187
Rotkiewicz, K., see J. Herbich 138 (1989) 105

Saik, V.O., see A.V. Koptyug 138 (1989) 173
Salzman, W.R., Semiclassical theory of microwave optical activity near resonance in asymmetric rotors 138 (1989) 25
Sampoli, M., see R. Frattini 138 (1989) 337
Shlihta, G.A., see E.A. Silinsh 138 (1989) 347
Silinsh, E.A., G.A. Shlihta and A.J. Jurgis, A model description of charge carrier transport phenomena in organic molecular crystals. I. Polyacene crystals 138 (1989) 347
Stoeckel, F., see A. Campargue 138 (1989) 405
Stoll, H., see E. Czuchaj 138 (1989) 303
Stolte, S., see E.W. Kuipers 138 (1989) 451
Storozhev, A.V., Nonresonance effects in the binary relaxation theory 138 (1989) 81

Tamai, N., see M. Furukawa 138 (1989) 423
Taylor, A.G., A.C. Jones and D. Phillips, Spectroscopy and structure of the jet-cooled carbazole dimer 138 (1989) 413
Tenner, M.G., see E.W. Kuipers 138 (1989) 451
Thibodeau, D.L., J.A. Koningstein and L.V. Haley, Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro 138 (1989) 265
Thulstrup, E.W., see J. Herbich 138 (1989) 105

Vallauri, R., see R. Frattini 138 (1989) 337

Waluk, J., see J. Herbich 138 (1989) 105
Wasada, H. and K. Hirao, Computational studies of satellite peaks of the inner-valence ionization of C_2H_4, C_2H_2 and H_2S using the SAC CI method 138 (1989) 277
Wild, U.P., see K. Palewska 138 (1989) 115
Williams, G.M., see S. Xia 138 (1989) 255
Wu, X.J., see J.R. Cao 138 (1989) 377

Xia, S., G.M. Williams and N.M. Edelstein, Contributions from the energy level structure of the $4f^{11}5d^1$ intermediate configuration to the electronic Raman scattering intensities of $TmPO_4$ 138 (1989) 255

Yamazaki, I., see M. Furukawa 138 (1989) 423

Zhang, J.M., see J.R. Cao 138 (1989) 377
Zhang, Y. and D.M. Hanson, Transition stress and configuration interaction for diatomic molecules 138 (1989) 71
Zhong, X., see J.R. Cao 138 (1989) 377
Zhu, Q.H., see J.R. Cao 138 (1989) 377

LIST OF SUBJECTS

1 METHODS

1.1 Theoretical

1.1.1 Group theory and algebras
1.1.2 Classical mechanics *
1.1.3 Quantized field theory
1.1.4 Many body and quasiparticle approaches *
1.1.5 Coupling schemes and perturbative treatments *
1.1.6 Relativistic quantum mechanics
1.1.7 Transport quantum mechanics
1.1.8 Equilibrium statistical mechanics
1.1.9 Statistical mechanics of stationary states
1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories
1.1.11 Ab initio schemes for stationary properties *
1.1.12 Computational and simulation methods *
1.1.13 Molecular dynamics and scattering theory *

1.2 Experimental

1.2.1 Magnetic resonances *
1.2.2 Cyclotron resonance
1.2.3 Microwave spectroscopy
1.2.4 Infrared spectroscopy *
1.2.5 Raman spectroscopy *
1.2.6 Visible and UV spectroscopy *
1.2.7 Fluorescence spectroscopy *
1.2.8 Photoelectron and Auger spectroscopy *
1.2.9 X-ray spectroscopy
1.2.10 Electron impact spectroscopy *
1.2.11 Laser methods *
1.2.12 Picosecond spectroscopy *
1.2.13 Non-linear optical spectroscopy
1.2.14 Synchrotron spectroscopies *
1.2.15 Coherent optical spectroscopy
1.2.16 Optical pumping *
1.2.17 Multiple resonance spectroscopy
1.2.18 Optoacoustic spectroscopy *
1.2.19 Atomic and molecular beam techniques *
1.2.20 Time-resolved experiments *
1.2.21 Mass spectrometry
1.2.22 Radiolysis *
1.2.23 Mössbauer spectroscopy
1.2.24 X-ray, electron and neutron diffraction
1.2.25 Neutron scattering *
1.2.26 Light scattering *
1.2.27 Field emission and field ionization
1.2.28 Measurement of macroscopic variables *

2 OBJECTS

2.1 Bulk systems

2.1.1 Gases *
2.1.2 Supersonic beams *
2.1.3 Liquids neat *
2.1.4 Liquid mixtures and solutions *
2.1.5 Crystals *
2.1.5.1 neat *
2.1.5.2 mixed
2.1.6 Glasses
2.1.7 Liquid crystals
2.1.8 Polymers *
2.1.9 Semiconductors
2.1.10 Metals and alloys
2.1.11 Thin films
2.1.12 Surfaces *
2.1.13 Low-dimensional materials
2.1.14 Dielectrics *
2.1.15 Plasmas
2.1.16 Biological systems *

2.2 Microscopic systems

2.2.1 Atoms *
2.2.2 Molecules (neutral and ionic) *
2.2.2.1 diatomic *
2.2.2.2 small polyatomics *
2.2.2.3 aromatics *
2.2.2.4 other large
2.2.2.5 polymeric and biological
2.2.3 Molecular aggregates *
2.2.3.1 dimers *
2.2.3.2 van der Waals molecules
2.2.3.3 clusters *
2.2.3.4 complexes *
2.2.4 Free radicals (including hydronium and muonium) *
2.2.5 Quasiparticles (including excitons) *
2.2.6 Defects and impurities *
2.2.7 Ions and charge carriers *

* Denotes subjects covered in this volume

3 PHENOMENA

3.1 Molecular structure *
3.2 Vibrations and rotations of molecules *
3.3 Electronic structure and states *
3.4 Electric and magnetic properties *
3.5 Spin splittings
3.6 Optical activity *
3.7 Molecular interactions *
3.8 Spectral bandshapes and intensities *
3.9 Coupling of electronic and nuclear motion
3.10 Energy transfer processes *
3.11 Molecular photophysical processes *
3.12 Intramolecular dynamics
3.12.1 radiationless transitions
3.12.2 vibrational energy redistribution (including vibrational dissociation)
3.13 Luminescence spectra, yields and lifetimes *
3.14 Coherence loss processes
3.15 Non-linear responses (including optical) *
3.16 Multiphoton phenomena *
3.17 Reactions (including dissociation) *
3.17.1 gas phase *
3.17.2 condensed phase *
3.17.3 photochemical *
3.18 Tunnelling *
3.19 Electron transfer *
3.20 Positron annihilation
3.21 Ionization (including Rydberg states) *
3.22 Molecular motion (including diffusive) *
3.23 Isotopic effects
3.24 Fluctuations and noise
3.25 Collective motion and excitations
3.26 Surface effects and catalysis *
3.27 Thermodynamic and transport properties
3.28 Structure of solids and liquids *
3.29 Critical phenomena
3.30 Phase transitions

SUBJECT INDEX TO VOLUME 138

METHODS

Theoretical

Classical mechanics

Dielectric theory of weak charge-transfer crystals. III. Dipole moments, R.W. Munn and R.J. Phillips 138 (1989) 223

Many body and quasiparticle approaches

Charge transfer effects in the pressure dependence of the ultraviolet absorption spectra of polyacene crystals, P. Petelenz 138 (1989) 35
Ab initio study of the outer valence ionization potentials and electron affinities of non-conjugated π-electron cyclic systems, V. Galasso 138 (1989) 231

Coupling schemes and perturbative treatments

Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model, M. Kamiya 138 (1989) 11
Semiclassical theory of microwave optical activity near resonance in asymmetric rotors, W.R. Salzman 138 (1989) 25
Nonresonance effects in the binary relaxation theory, A.V. Storozhev 138 (1989) 81
Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 123
Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 139
The nature of molecular vibrations selected by various excitation processes, H.G. Kjaergaard and O.S. Mortensen 138 (1989) 237
Semiclassical coupled state sudden approximation for multipole cross sections in atom–diatom systems, C. Nyeland and G.D. Billing 138 (1989) 245
Contributions from the energy level structure of the $4f^{11}5d^1$ intermediate configuration to the electronic Raman scattering intensities of $TmPO_4$, S. Xia, G.M. Williams and N.M. Edelstein 138 (1989) 255
Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265

Ab initio schemes for stationary properties

Transition stress and configuration interaction for diatomic molecules, Y. Zhang and D.M. Hanson 138 (1989) 71
The low-lying electronic states of indium trimer, P.Y. Feng and K. Balasubramanian 138 (1989) 89

Ab initio CI calculations on the molecular structure of Sn_2H_4 isomers, A. Márquez, G.G. González and J. Fernández Sanz 138 (1989) 99
HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN_2H_2 energy hypersurface, C. Guimon, S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo 138 (1989) 157
Theoretical study of the generalized oscillator strength for the $A\,^1B_1$–$X\,^1A_1$ transition in the water molecule, K. Bhanuprakash, P. Chandra, C. Chabalowski and R.J. Buenker 138 (1989) 215
Computational studies of satellite peaks of the inner-valence ionization of C_2H_4, C_2H_2 and H_2S using the SAC CI method, H. Wasada and K. Hirao 138 (1989) 277
A theoretical study of the C_2H, C_2F and C_2Cl radicals and their positive ions, A. Largo and C. Barrientos 138 (1989) 291
Semi-local pseudopotential calculations for the potential energies of the CaHe and CaNe systems, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 138 (1989) 303
Pseudopotential MRD CI calculations of nickel-containing molecules. II. The electronic $^1\Sigma^+$ ground state and 20 low-lying excited states of the NiSi molecule, H. Haberlandt 138 (1989) 315
A computation procedure for the dispersion component of the interaction energy in continuum solute–solvent models, M.A. Aguilar and F.J. Olivares del Valle 138 (1989) 327

Computational and simulation methods

Transition moment directions and molecular structure of some *p*-cyano-N,N-dimethylaniline derivatives, J. Herbich, K. Rotkiewicz, J. Waluk, B. Andresen and E.W. Thulstrup 138 (1989) 105
A theoretical study of the C_2H, C_2F and C_2Cl radicals and their positive ions, A. Largo and C. Barrientos 138 (1989) 291
Analysis of the orientational order induced by different potential models for CO_2, R. Frattini, D. Gazzillo, M. Sampoli and R. Vallauri 138 (1989) 337
A model description of charge carrier transport phenomena in organic molecular crystals. I. Polyacene crystals, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 138 (1989) 347
An MNDO calculational study of selected oxazine, thiazine and oxazone dyes, G.J. Blanchard 138 (1989) 365

Molecular dynamics and scattering theory

Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model, M. Kamiya 138 (1989) 11
Optimal trajectory approach in the theory of photodissociation of thermally excited molecules, E.E. Nikitin and M.Ya. Ovchinnikova 138 (1989) 45
Infrared and molecular dynamics study of reorientational relaxation of liquid acetonitrile, S. Hashimoto, T. Ohba and S. Ikawa 138 (1989) 63
Semiclassical coupled state sudden approximation for multipole cross sections in atom–diatom systems, C. Nyeland and G.D. Billing 138 (1989) 245
Photofragmentation of vinyl iodide at 248 nm. Heat of formation of vinyl radical, J.R. Cao, J.M. Zhang, X. Zhong, Y.H. Huang, W.Q. Fang, X.J. Wu and Q.H. Zhu 138 (1989) 377

Experimental

Magnetic resonances

Spin-locking in concentration-narrowed OD ESR spectra, A.V. Koptyug, V.O. Saik, O.A. Anisimov and Yu.N. Molin 138 (1989) 173

Methyl tunnelling in tiglic acid and 2-methyl-2-butene, A.J. Horsewill, R.M. Green and A.M. Alsanoosi 138 (1989) 179
Time-resolved microwave-induced optical nuclear polarization, D. Henrich, H. Brunner, R.H. Fritsch and K.H. Hausser 138 (1989) 203
A relaxation time study of molecular motion in trimethylolpropane triacrylate and trimethylolpropane trimethacrylate, J.W. Harrell Jr. and S.J. Ahuja 138 (1989) 383

Infrared spectroscopy
Infrared and molecular dynamics study of reorientational relaxation of liquid acetonitrile, S. Hashimoto, T. Ohba and S. Ikawa 138 (1989) 63
Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide, J.R. Durig, H.V. Phan and T.S. Little 138 (1989) 391
High-resolution overtone spectroscopy of SiH_4 and $SiHD_3$ ($\Delta v_{SiH}=6$) and CH_4 ($\Delta v_{CH}=5$), A. Campargue, M. Chenevier and F. Stoeckel 138 (1989) 405

Raman spectroscopy
The nature of molecular vibrations selected by various excitation processes, H.G. Kjaergaard and O.S. Mortensen 138 (1989) 237
Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265
Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide, J.R. Durig, H.V. Phan and T.S. Little 138 (1989) 391

Visible and UV spectroscopy
Charge transfer effects in the pressure dependence of the ultraviolet absorption spectra of polyacene crystals, P. Petelenz 138 (1989) 35
Transition moment directions and molecular structure of some *p*-cyano-N,N-dimethylaniline derivatives, J. Herbich, K. Rotkiewicz, J. Waluk, B. Andresen and E.W. Thulstrup 138 (1989) 105
Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 123
Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 139
The nature of molecular vibrations selected by various excitation processes, H.G. Kjaergaard and O.S. Mortensen 138 (1989) 237
Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265
High-resolution overtone spectroscopy of SiH_4 and $SiHD_3$ ($\Delta v_{SiH}=6$) and CH_4 ($\Delta v_{CH}=5$), A. Campargue, M. Chenevier and F. Stoeckel 138 (1989) 405

Fluorescence spectroscopy
Intramolecular electron transfer in viscous solution, P. Finckh, H. Heitele and M.E. Michel-Beyerle 138 (1989) 1
Spectroscopic evidence for the coexistence of two stereoisomers of tetrabenzonaphthalene in Shpol'skii-type matrices at 4.2 K, K. Palewska, E.C. Meister and U.P. Wild 138 (1989) 115
Spectroscopy and structure of the jet-cooled carbazole dimer, A.G. Taylor, A.C. Jones and D. Phillips 138 (1989) 413

Branching of exciton relaxation to the free and self-trapped exciton states, M. Furukawa, K. Mizuno, A. Matsui, N. Tamai and I. Yamazaki 138 (1989) 423

Photoelectron and Auger spectroscopy

HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN_2H_2 energy hypersurface, C. Guimon, S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo 138 (1989) 157

Ab initio study of the outer valence ionization potentials and electron affinities of non-conjugated π-electron cyclic systems, V. Galasso 138 (1989) 231

Electron impact spectroscopy

About the double ionization of ammonia and carbon dioxide. A comparison between photoionization and electron impact, R. Locht, M. Davister, W. Denzer, H.W. Jochims and H. Baumgärtel 138 (1989) 433

Laser methods

Time-resolved molecular chemiluminescence investigations of SrO following pulsed dye-laser generation of $Sr(5s5p(^3P_J))$ in the presence of N_2O, D. Husain and G. Roberts 138 (1989) 187

Photofragmentation of vinyl iodide at 248 nm. Heat of formation of vinyl radical, J.R. Cao, J.M. Zhang, X. Zhong, Y.H. Huang, W.Q. Fang, X.J. Wu and Q.H. Zhu 138 (1989) 377

High-resolution overtone spectroscopy of SiH_4 and $SiHD_3$ ($\Delta v_{SiH}=6$) and CH_4 ($\Delta v_{CH}=5$), A. Campargue, M. Chenevier and F. Stoeckel 138 (1989) 405

Picosecond spectroscopy

Branching of exciton relaxation to the free and self-trapped exciton states, M. Furukawa, K. Mizuno, A. Matsui, N. Tamai and I. Yamazaki 138 (1989) 423

Synchrotron spectroscopies

About the double ionization of ammonia and carbon dioxide. A comparison between photoionization and electron impact, R. Locht, M. Davister, W. Denzer, H.W. Jochims and H. Baumgärtel 138 (1989) 433

Optical pumping

Multiphoton absorption and luminescence of chromyl chloride, M. Ivanco, D.K. Evans and R.D. McAlpine 138 (1989) 441

Optoacoustic spectroscopy

Multiphoton absorption and luminescence of chromyl chloride, M. Ivanco, D.K. Evans and R.D. McAlpine 138 (1989) 441

Atomic and molecular beam techniques

Photofragmentation of vinyl iodide at 248 nm. Heat of formation of vinyl radical, J.R. Cao, J.M. Zhang, X. Zhong, Y.H. Huang, W.Q. Fang, X.J. Wu and Q.H. Zhu 138 (1989) 377

Dependence of the NO/Ag(111) trapping probability on molecular orientation, E.W. Kuipers, M.G. Tenner, A.W. Kleyn and S. Stolte 138 (1989) 451

Time-resolved experiments
Intramolecular electron transfer in viscous solution, P. Finckh, H. Heitele and M.E. Michel-Beyerle 138 (1989) 1
Time-resolved molecular chemiluminescence investigations of SrO following pulsed dye-laser generation of Sr(5s5p(^3P_J)) in the presence of N_2O, D. Husain and G. Roberts 138 (1989) 187

Radiolysis
Spin-locking in concentration-narrowed OD ESR spectra, A.V. Koptyug, V.O. Saik, O.A. Anisimov and Yu.N. Molin 138 (1989) 173

Neutron scattering
Methyl tunnelling in tiglic acid and 2-methyl-2-butene, A.J. Horsewill, R.M. Green and A.M. Alsanoosi 138 (1989) 179

Light scattering
Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model, M. Kamiya 138 (1989) 11

Measurement of macroscopic variables
A model description of charge carrier transport phenomena in organic molecular crystals. I. Polyacene crystals, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 138 (1989) 347

OBJECTS

Bulk systems

Gases
Nonresonance effects in the binary relaxation theory, A.V. Storozhev 138 (1989) 81
HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN_2H_2 energy hypersurface, C. Guimon, S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo 138 (1989) 157
Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide, J.R. Durig, H.V. Phan and T.S. Little 138 (1989) 391
About the double ionization of ammonia and carbon dioxide. A comparison between photoionization and electron impact, R. Locht, M. Davister, W. Denzer, H.W. Jochims and H. Baumgärtel 138 (1989) 433

Supersonic beams
Spectroscopy and structure of the jet-cooled carbazole dimer, A.G. Taylor, A.C. Jones and D. Phillips 138 (1989) 413

Liquids neat
Infrared and molecular dynamics study of reorientational relaxation of liquid acetonitrile, S. Hashimoto, T. Ohba and S. Ikawa 138 (1989) 63
A relaxation time study of molecular motion in trimethylolpropane triacrylate and trimethylolpropane trimethacrylate, J.W. Harrell Jr. and S.J. Ahuja 138 (1989) 383
Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide, J.R. Durig, H.V. Phan and T.S. Little 138 (1989) 391

Liquid mixtures and solutions
Spin-locking in concentration-narrowed OD ESR spectra, A.V. Koptyug, V.O. Saik, O.A. Anisimov and Yu.N. Molin 138 (1989) 173
A computation procedure for the dispersion component of the interaction energy in continuum solute–solvent models, M.A. Aguilar and F.J. Olivares del Valle 138 (1989) 327

Crystals
Dielectric theory of weak charge-transfer crystals. III. Dipole moments, R.W. Munn and R.J. Phillips 138 (1989) 223
A model description of charge carrier transport phenomena in organic molecular crystals. I. Polyacene crystals, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 138 (1989) 347
Branching of exciton relaxation to the free and self-trapped exciton states, M. Furukawa, K. Mizuno, A. Matsui, N. Tamai and I. Yamazaki 138 (1989) 423

–neat
Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 123
Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 139

Polymers
Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model, M. Kamiya 138 (1989) 11

Surfaces
Dependence of the NO/Ag(111) trapping probability on molecular orientation, E.W. Kuipers, M.G. Tenner, A.W. Kleyn and S. Stolte 138 (1989) 451

Dielectrics
Dielectric theory of weak charge-transfer crystals. III. Dipole moments, R.W. Munn and R.J. Phillips 138 (1989) 223

Biological systems
Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265

Microscopic systems

Atoms
Time-resolved molecular chemiluminescence investigations of SrO following pulsed dye-laser generation of $Sr(5s5p(^3P_J))$ in the presence of N_2O, D. Husain and G. Roberts 138 (1989) 187

Molecules (neutral and ionic)
Nonresonance effects in the binary relaxation theory, A.V. Storozhev 138 (1989) 81
The nature of molecular vibrations selected by various excitation processes, H.G. Kjaergaard and O.S. Mortensen 138 (1989) 237

–diatomic

Transition stress and configuration interaction for diatomic molecules, Y. Zhang and D.M. Hanson 138 (1989) 71

Semi-local pseudopotential calculations for the potential energies of the CaHe and CaNe systems, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 138 (1989) 303

Pseudopotential MRD CI calculations of nickel-containing molecules. II. The electronic $^1\Sigma^+$ ground state and 20 low-lying excited states of the NiSi molecule, H. Haberlandt 138 (1989) 315

Dependence of the NO/Ag(111) trapping probability on molecular orientation, E.W. Kuipers, M.G. Tenner, A.W. Kleyn and S. Stolte 138 (1989) 451

–small polyatomics

Semiclassical theory of microwave optical activity near resonance in asymmetric rotors, W.R. Salzman 138 (1989) 25

Optimal trajectory approach in the theory of photodissociation of thermally excited molecules, E.E. Nikitin and M.Ya. Ovchinnikova 138 (1989) 45

HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN_2H_2 energy hypersurface, C. Guimon, S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo 138 (1989) 157

Theoretical study of the generalized oscillator strength for the $A\,^1B_1$–$X\,^1A_1$ transition in the water molecule, K. Bhanuprakash, P. Chandra, C. Chabalowski and R.J. Buenker 138 (1989) 215

Ab initio study of the outer valence ionization potentials and electron affinities of non-conjugated π-electron cyclic systems, V. Galasso 138 (1989) 231

Computational studies of satellite peaks of the inner-valence ionization of C_2H_4, C_2H_2 and H_2S using the SAC CI method, H. Wasada and K. Hirao 138 (1989) 277

Analysis of the orientational order induced by different potential models for CO_2, R. Frattini, D. Gazzillo, M. Sampoli and R. Vallauri 138 (1989) 337

Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide, J.R. Durig, H.V. Phan and T.S. Little 138 (1989) 391

About the double ionization of ammonia and carbon dioxide. A comparison between photoionization and electron impact, R. Locht, M. Davister, W. Denzer, H.W. Jochims and H. Baumgärtel 138 (1989) 433

–aromatics

Spectroscopic evidence for the coexistence of two stereoisomers of tetrabenzonaphthalene in Shpol'skii-type matrices at 4.2 K, K. Palewska, E.C. Meister and U.P. Wild 138 (1989) 115

Spin-locking in concentration-narrowed OD ESR spectra, A.V. Koptyug, V.O. Saik, O.A. Anisimov and Yu.N. Molin 138 (1989) 173

A model description of charge carrier transport phenomena in organic molecular crystals. I. Polyacene crystals, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 138 (1989) 347

An MNDO calculational study of selected oxazine, thiazine and oxazone dyes, G.J. Blanchard 138 (1989) 365

Molecular aggregates

Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model, M. Kamiya 138 (1989) 11

A computation procedure for the dispersion component of the interaction energy in continuum solute–solvent models, M.A. Aguilar and F.J. Olivares del Valle 138 (1989) 327

–dimers
Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265
Spectroscopy and structure of the jet-cooled carbazole dimer, A.G. Taylor, A.C. Jones and D. Phillips 138 (1989) 413

–clusters
The low-lying electronic states of indium trimer, P.Y. Feng and K. Balasubramanian 138 (1989) 89

–complexes
Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 123
Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 139

Free radicals (including hydronium and muonium)
Photofragmentation of vinyl iodide at 248 nm. Heat of formation of vinyl radical, J.R. Cao, J.M. Zhang, X. Zhong, Y.H. Huang, W.Q. Fang, X.J. Wu and Q.H. Zhu 138 (1989) 377

Quasiparticles (including excitons)
Charge transfer effects in the pressure dependence of the ultraviolet absorption spectra of polyacene crystals, P. Petelenz 138 (1989) 35
Branching of exciton relaxation to the free and self-trapped exciton states, M. Furukawa, K. Mizuno, A. Matsui, N. Tamai and I. Yamazaki 138 (1989) 423

Defects and impurities
Contributions from the energy level structure of the $4f^{11}5d^1$ intermediate configuration to the electronic Raman scattering intensities of $TmPO_4$, S. Xia, G.M. Williams and N.M. Edelstein 138 (1989) 255

Ions and charge carriers
Dielectric theory of weak charge-transfer crystals. III. Dipole moments, R.W. Munn and R.J. Phillips 138 (1989) 223

PHENOMENA

Molecular structure
Transition stress and configuration interaction for diatomic molecules, Y. Zhang and D.M. Hanson 138 (1989) 71
The low-lying electronic states of indium trimer, P.Y. Feng and K. Balasubramanian 138 (1989) 89
Spectroscopic evidence for the coexistence of two stereoisomers of tetrabenzonaphthalene in Shpol'skii-type matrices at 4.2 K, K. Palewska, E.C. Meister and U.P. Wild 138 (1989) 115
A theoretical study of the C_2H, C_2F and C_2Cl radicals and their positive ions, A. Largo and C. Barrientos 138 (1989) 291

Pseudopotential MRD CI calculations of nickel-containing molecules. II. The electronic $^1\Sigma^+$ ground state and 20 low-lying excited states of the NiSi molecule, H. Haberlandt 138 (1989) 315

Vibrations and rotations of molecules

Methyl tunnelling in tiglic acid and 2-methyl-2-butene, A.J. Horsewill, R.M. Green and A.M. Alsanoosi 138 (1989) 179

The nature of molecular vibrations selected by various excitation processes, H.G. Kjaergaard and O.S. Mortensen 138 (1989) 237

Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265

Conformational stability, barriers to internal rotation and vibrational assignments of fluoroacetyl bromide, J.R. Durig, H.V. Phan and T.S. Little 138 (1989) 391

High-resolution overtone spectroscopy of SiH_4 and $SiHD_3$ ($\Delta\nu_{SiH}=6$) and CH_4 ($\Delta\nu_{CH}=5$), A. Campargue, M. Chenevier and F. Stoeckel 138 (1989) 405

Electronic structure and states

Charge transfer effects in the pressure dependence of the ultraviolet absorption spectra of polyacene crystals, P. Petelenz 138 (1989) 35

Transition stress and configuration interaction for diatomic molecules, Y. Zhang and D.M. Hanson 138 (1989) 71

The low-lying electronic states of indium trimer, P.Y. Feng and K. Balasubramanian 138 (1989) 89

Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 123

Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 139

Theoretical study of the generalized oscillator strength for the $A\,^1B_1$–$X\,^1A_1$ transition in the water molecule, K. Bhanuprakash, P. Chandra, C. Chabalowski and R.J. Buenker 138 (1989) 215

Ab initio study of the outer valence ionization potentials and electron affinities of non-conjugated π-electron cyclic systems, V. Galasso 138 (1989) 231

Contributions from the energy level structure of the $4f^{11}5d^1$ intermediate configuration to the electronic Raman scattering intensities of $TmPO_4$, S. Xia, G.M. Williams and N.M. Edelstein 138 (1989) 255

Computational studies of satellite peaks of the inner-valence ionization of C_2H_4, C_2H_2 and H_2S using the SAC CI method, H. Wasada and K. Hirao 138 (1989) 277

A theoretical study of the C_2H, C_2F and C_2Cl radicals and their positive ions, A. Largo and C. Barrientos 138 (1989) 291

Semi-local pseudopotential calculations for the potential energies of the CaHe and CaNe systems, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 138 (1989) 303

Pseudopotential MRD CI calculations of nickel-containing molecules. II. The electronic $^1\Sigma^+$ ground state and 20 low-lying excited states of the NiSi molecule, H. Haberlandt 138 (1989) 315

An MNDO calculational study of selected oxazine, thiazine and oxazone dyes, G.J. Blanchard 138 (1989) 365

Spectroscopy and structure of the jet-cooled carbazole dimer, A.G. Taylor, A.C. Jones and D. Phillips 138 (1989) 413

Electric and magnetic properties
Dielectric theory of weak charge-transfer crystals. III. Dipole moments, R.W. Munn and R.J. Phillips 138 (1989) 223

Optical activity
Theoretical investigation on the optical bandshape properties of chromophore aggregates by use of the incoherent dynamic interaction model, M. Kamiya 138 (1989) 11
Semiclassical theory of microwave optical activity near resonance in asymmetric rotors, W.R. Salzman 138 (1989) 25

Molecular interactions
Nonresonance effects in the binary relaxation theory, A.V. Storozhev 138 (1989) 81
Crystal-field energy levels and transition line strengths of neodymium in trigonal $Na_3[Nd(oxydiacetate)_3]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 123
Semiclassical coupled state sudden approximation for multipole cross sections in atom–diatom systems, C. Nyeland and G.D. Billing 138 (1989) 245
A computation procedure for the dispersion component of the interaction energy in continuum solute–solvent models, M.A. Aguilar and F.J. Olivares del Valle 138 (1989) 327
Spectroscopy and structure of the jet-cooled carbazole dimer, A.G. Taylor, A.C. Jones and D. Phillips 138 (1989) 413

Spectral bandshapes and intensities
Infrared and molecular dynamics study of reorientational relaxation of liquid acetonitrile, S. Hashimoto, T. Ohba and S. Ikawa 138 (1989) 63
Nonresonance effects in the binary relaxation theory, A.V. Storozhev 138 (1989) 81
Parametric analysis of f–f transition intensities in trigonal $Na_3[Nd(oxydiacetate_3)]\cdot 2NaClO_4\cdot 6H_2O$, P.S. May, C.K. Jayasankar and F.S. Richardson 138 (1989) 139
Theoretical study of the generalized oscillator strength for the $A\,^1B_1$–$X\,^1A_1$ transition in the water molecule, K. Bhanuprakash, P. Chandra, C. Chabalowski and R.J. Buenker 138 (1989) 215

Energy transfer processes
Time-resolved molecular chemiluminescence investigations of SrO following pulsed dye-laser generation of $Sr(5s5p(^3P_J))$ in the presence of N_2O, D. Husain and G. Roberts 138 (1989) 187
Semiclassical coupled state sudden approximation for multipole cross sections in atom–diatom systems, C. Nyeland and G.D. Billing 138 (1989) 245
Dependence of the NO/Ag(111) trapping probability on molecular orientation, E.W. Kuipers, M.G. Tenner, A.W. Kleyn and S. Stolte 138 (1989) 451

Molecular photophysical processes
Optimal trajectory approach in the theory of photodissociation of thermally excited molecules, E.E. Nikitin and M.Ya. Ovchinnikova 138 (1989) 45
Resonant vibrational light scattering spectrum of a pair of chlorophyll **a** in vitro, D.L. Thibodeau, J.A. Koningstein and L.V. Haley 138 (1989) 265
Multiphoton absorption and luminescence of chromyl chloride, M. Ivanco, D.K. Evans and R.D. McAlpine 138 (1989) 441

Luminescence spectra, yields and lifetimes
Branching of exciton relaxation to the free and self-trapped exciton states, M. Furukawa, K. Mizuno, A. Matsui, N. Tamai and I. Yamazaki 138 (1989) 423
Multiphoton absorption and luminescence of chromyl chloride, M. Ivanco, D.K. Evans and R.D. McAlpine 138 (1989) 441

Non-linear responses (including optical)
Spin-locking in concentration-narrowed OD ESR spectra, A.V. Koptyug, V.O. Saik, O.A. Anisimov and Yu.N. Molin 138 (1989) 173

Multiphoton phenomena
Multiphoton absorption and luminescence of chromyl chloride, M. Ivanco, D.K. Evans and R.D. McAlpine 138 (1989) 441

Reactions (including dissociation)

–gas phase
HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN_2H_2 energy hypersurface, C. Guimon, S. Khayar, F. Gracian, M. Begtrup and G. Pfister-Guillouzo 138 (1989) 157
Time-resolved molecular chemiluminescence investigations of SrO following pulsed dye-laser generation of $Sr(5s5p(^3P_J))$ in the presence of N_2O, D. Husain and G. Roberts 138 (1989) 187

–condensed phase
Intramolecular electron transfer in viscous solution, P. Finckh, H. Heitele and M.E. Michel-Beyerle 138 (1989) 1

–photochemical
Optimal trajectory approach in the theory of photodissociation of thermally excited molecules, E.E. Nikitin and M.Ya. Ovchinnikova 138 (1989) 45
Photofragmentation of vinyl iodide at 248 nm. Heat of formation of vinyl radical, J.R. Cao, J.M. Zhang, X. Zhong, Y.H. Huang, W.Q. Fang, X.J. Wu and Q.H. Zhu 138 (1989) 377

Tunnelling
Methyl tunnelling in tiglic acid and 2-methyl-2-butene, A.J. Horsewill, R.M. Green and A.M. Alsanoosi 138 (1989) 179

Electron transfer
Intramolecular electron transfer in viscous solution, P. Finckh, H. Heitele and M.E. Michel-Beyerle 138 (1989) 1
Charge transfer effects in the pressure dependence of the ultraviolet absorption spectra of polyacene crystals, P. Petelenz 138 (1989) 35
A model description of charge carrier transport phenomena in organic molecular crystals. I. Polyacene crystals, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 138 (1989) 347

Ionization (including Rydberg states)
Theoretical study of the generalized oscillator strength for the $A\,^1B_1$–$X\,^1A_1$ transition in the water molecule, K. Bhanuprakash, P. Chandra, C. Chabalowski and R.J. Buenker 138 (1989) 215

Computational studies of satellite peaks of the inner-valence ionization of C_2H_4, C_2H_2 and H_2S using the SAC CI method, H. Wasada and K. Hirao 138 (1989) 277
About the double ionization of ammonia and carbon dioxide. A comparison between photoionization and electron impact, R. Locht, M. Davister, W. Denzer, H.W. Jochims and H. Baumgärtel 138 (1989) 433

Molecular motion (including diffusive)
Infrared and molecular dynamics study of reorientational relaxation of liquid acetonitrile, S. Hashimoto, T. Ohba and S. Ikawa 138 (1989) 63
Methyl tunnelling in tiglic acid and 2-methyl-2-butene, A.J. Horsewill, R.M. Green and A.M. Alsanoosi 138 (1989) 179
A relaxation time study of molecular motion in trimethylolpropane triacrylate and trimethylolpropane trimethacrylate, J.W. Harrell Jand S.J. Ahuja 138 (1989) 383

Surface effects and catalysis
Dependence of the NO/Ag(111) trapping probability on molecular orientation, E.W. Kuipers, M.G. Tenner, A.W. Kleyn and S. Stolte 138 (1989) 451

Structure of solids and liquids
Analysis of the orientational order induced by different potential models for CO_2, R. Frattini, D. Gazzillo, M. Sampoli and R. Vallauri 138 (1989) 337